Resonant Soft-X-Ray Emission of Molecular Materials: Electronic Structure and Dynamics

J.-H. Guo*, Y. Luo†, A. Augustsson*, J.-E. Rubensson*, C. Såthe*, H. Ågren†, H. Siegbahn*, and J. Nordgren*

* Department of Physics, Uppsala University, Box 530, S-75121, Uppsala, Sweden

†Theoretical Chemistry, Royal Institute of Technology, Teknikringen 36, S-100 44, Stockholm, Sweden

With high resolution monochromatized synchrotron radiation excitations, resonant soft-x-ray emission (inelastic soft-x-ray scattering) has emerged as a new source of information about electronic structure and excitation dynamics. We present a series of experimental counts, including the studies of small molecules to demonstrate the selection rules of energy, momentum, and symmetry in the resonant soft-x-ray emission process. In a molecular system, such as C_{60}, C_{70}, benzene, and polymers, symmetry selection rules are established, and deviations from the selection rules are interpreted in terms of dynamical symmetry breaking. In the studies of -conjugated polymers, we find that the benzene-ring has a strong identity as building block in some of the conjugated polymers. The application of core spectroscopic methods to liquids has been hampered by the incompatibility of wet samples and high-vacuum conditions. We take advantage of the large photon attenuation length to perform the first soft-x-ray emission study of liquid water. Here we examine the influence of the intermolecular interaction on the local electronic structure. We find a strong involvement of a_1-symmetry valence states in the hydrogen bonding. The local electronic structure of water molecules, where one hydrogen bond is broken at the hydrogen site, is separately determined. Also the resonant measurements in $K_3[Fe(CN)_6]$ water solution reveal chemical-species-selected valence band features unique to those water molecules bonded to $[Fe(CN)_6]^{3+}$ clusters. The results illustrate the power of using soft-x-ray emission spectroscopy to study the electronic structure of liquids in general.

Presenting Author:
Name: Jinghua Guo
Title: Prof (choose one)
Affiliation (Organisation): Uppsala University
Address: Department of Physics, Uppsala University, Box 530, 751 21 Uppsala, Sweden
Tel: +46 18 4713561
Fax: +46 18 4713524
Email: jinghua@fysik.uu.se

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